Proxy App Usecases at Sandia

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Proxy App Usecases at Sandia

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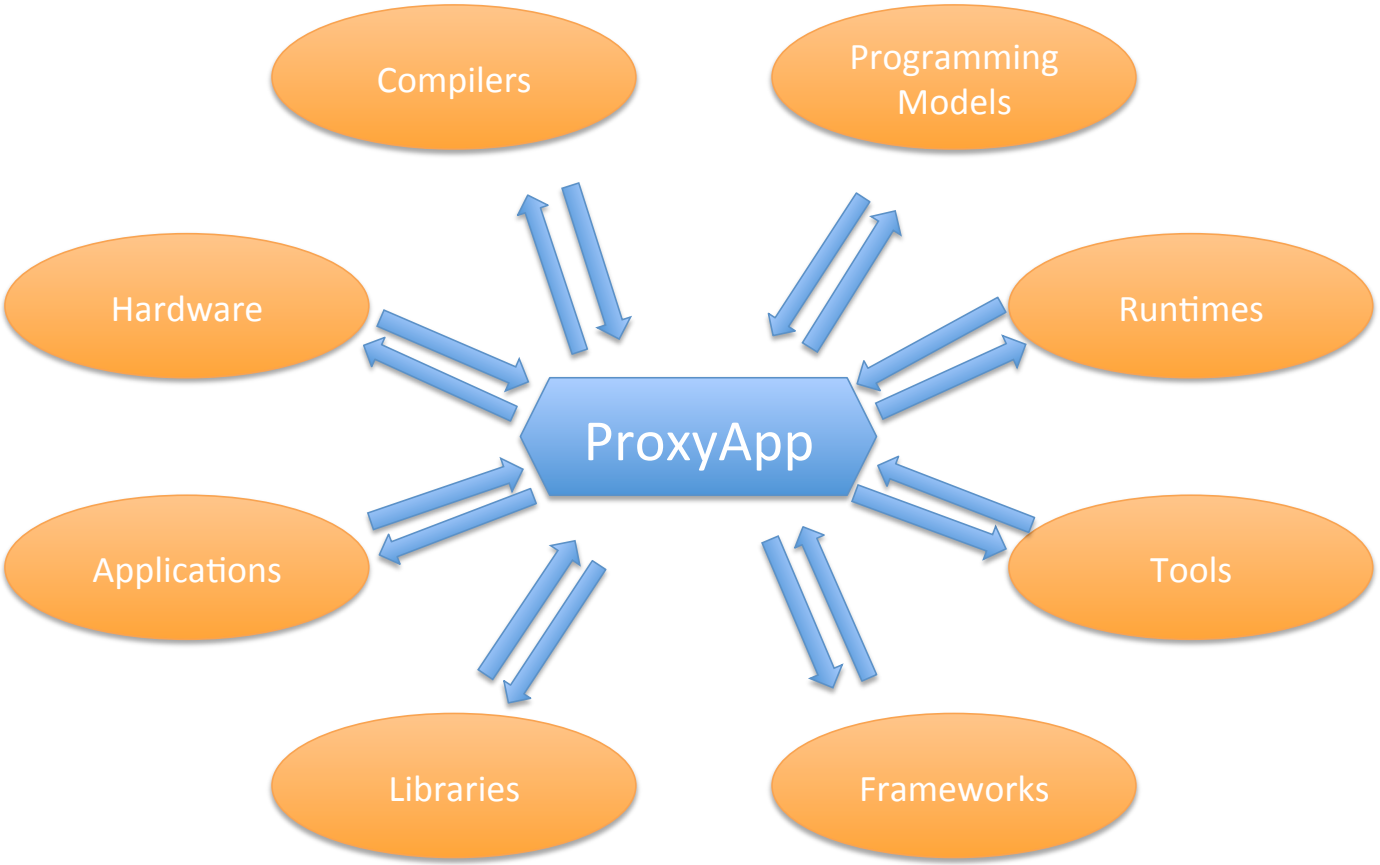
Proxy Apps: Connecting the Pieces



Phases of Proxy App Use

Evaluating Programming Models

- Starting 2011 use of proxy apps to experiment with on-node programming models
- MiniFE: 20+ variants in 10+ programming models (Serial,OpenMP,Cuda,OpenCL,Cilk,TBB,Kokkos,...)
- Use to inform development of Kokkos and perform comparisons with native programming models
- Now: evaluation of inter node tasking models

Develop Transition Strategies

- Prototype algorithms for thread scalability
- Develop and demonstrate incremental approach to adopt new architectures
- Use of miniDrivers to accelerate porting of libraries

Vendor collaboration

- Mini-apps are ideal for early hardware evaluation (simulators and early silicon)
- Utilized in procurements for benchmarks

Evaluating Programming Models

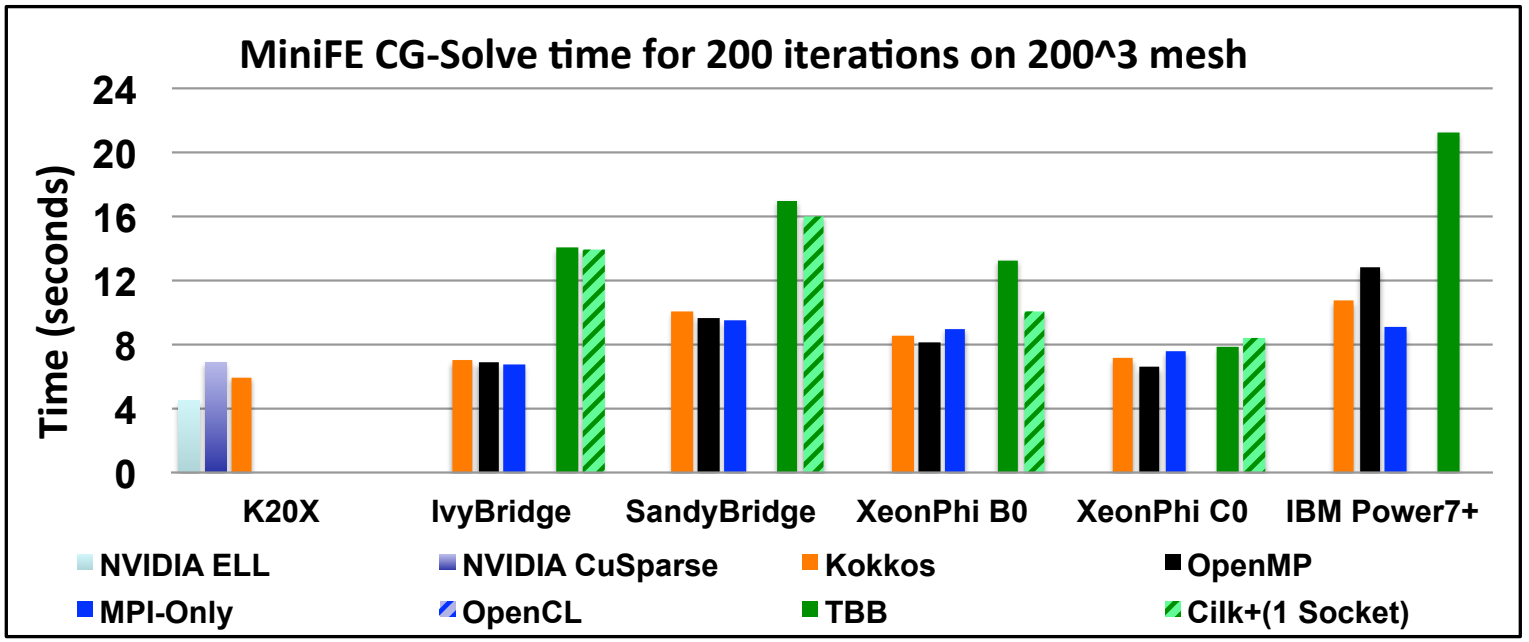
Ca. 2011:

- Becoming clear that medium term future will not allow MPI-only
- New programming models coming out seemingly every few months: Cuda, OpenCL, OpenACC, TBB, Cilk, C++AMP ...
- Which ones are viable? How do they perform? How portable are they? How hard to use?
- Not possible to evaluate in production codes: need miniApps to give space for rapid experimentation
- Start of DOE CoDesign centers and related miniApp efforts: Mantevo, ExMatEx, ExaCT, CESAR

Ca. 2014:

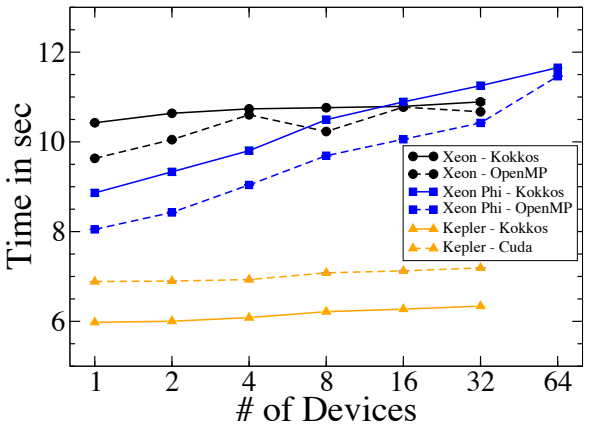
- Wide range of implementations are available, can run many miniApps on all hardware platforms.
- Understanding of strengths and weaknesses of different approaches exists
- Knowledge has been used to design new programming models for C++ (Raja, Kokkos)
- Using miniApps to validate new models (e.g. I. Karlin, et al. *"Lulesh programming model and performance ports overview."* Lawrence Livermore National Laboratory (LLNL), Livermore, CA, **Tech. Rep (2012)**.)

- Focus on simple Krylov solver (CG)
- Think of it as Sandia's Stream benchmark
- If this doesn't work well no point in going further
- Probably most variants of any MiniApp (30+)



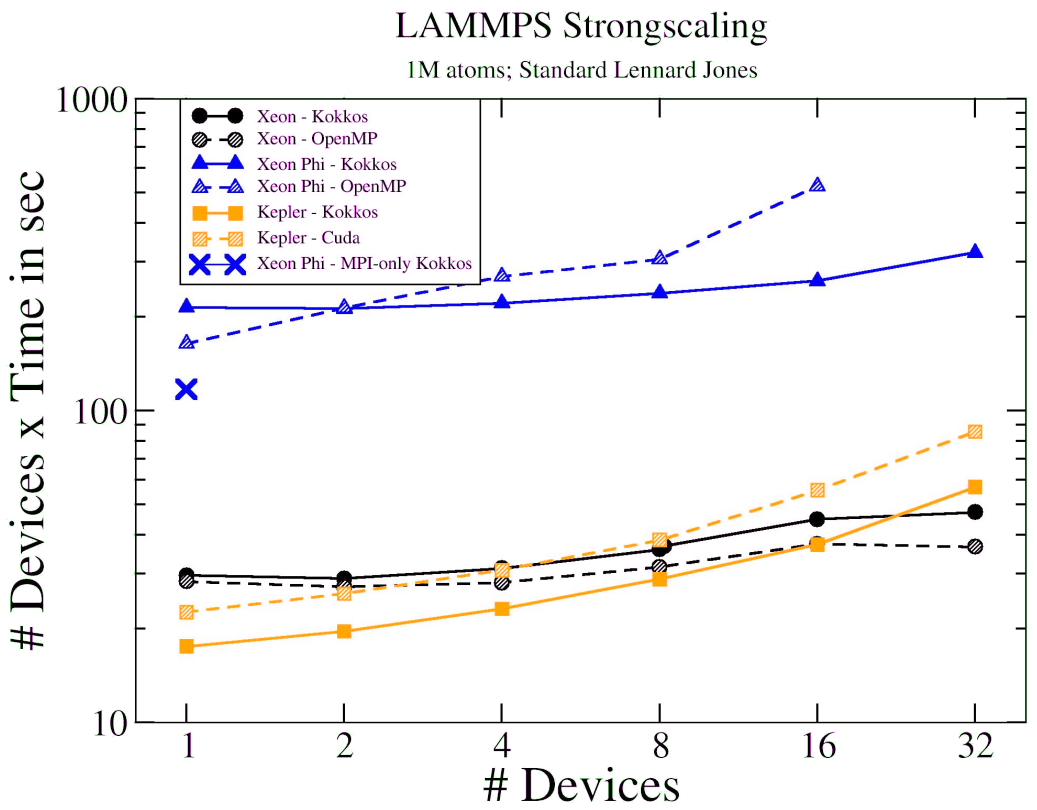
MiniMD - Prototyping a path forward for LAMMPS

- Direct connection to LAMMPS (same people, same code style, same algorithm)
- Challenging piece of code for compilers and architectures
- No single bottleneck, and sensitive to almost all performance characteristics of an architecture



MiniMD - Prototyping a path forward for LAMMPS

- Most of MiniMD's characteristics are perfectly reflected in LAMMPS
- But: Xeon Phi significantly different relative performance
- Reason are less gathers due to single atom type implementation of MiniMD



Renewed focus on task runtimes

- Dharma project at SNL California: evaluate different tasking models including Legion, Uintah and Charm++
- LLNL summer students ported miniApps for tasking frameworks
- LANL looking at Legion+Kokkos
- Interested in Resilience and Load-Balancing

Time is running out

- Current DOE leadership class machines get replaced in 2016 and 2018
- New platforms use XeonPhi (Trinity @ LANL/SNL, NERSC8 @ NERSC, ... @ ANL) or GPUs (Summit @ ORNL, Sierra @ LLNL)
- Threading is required for good performance
- Need to start porting now: Decisions have to be made
- Sandia: MPI + OpenMP and Kokkos; medium term Kokkos to get to Coral platforms

Guiding application teams

- Minimal threading experience in application teams
- Need to run education programs
- Need to develop guidelines for porting
- Incremental approaches necessary

- Part of a TriLab (LLNL,LANL,SNL) CoDesign Milestone
- Our take: demonstrate phases of adopting Kokkos aligned with machine lifecycle
- 5 Variants were written: Minimal CPU, Minimal GPU, Opt 1-3
- Demonstrate performance improvements related to necessary code changes

Developed Steps for Migrating Apps:

- Add `Kokkos::parallel_for` with capture by reference
- Mitigate write conflicts with atomics
- Capture by value
- Move data structures to use Kokkos allocations
- Introduce Multi-Dimensional Views with Layouts and Traits
- Use new algorithms where necessary

Initial introduction of Kokkos

- Support CPU like architectures only
- Replace loops with `parallel_for` and `parallel_reduce`
- Resolve write conflicts with atomic operations
- No change to data structures
- Not portable!

Adding parallel_for (34x)

```
//replace
for (Index_t i = 0; i < numElem; ++i) {
  ...
}
//with
Kokkos::parallel_for ( numElem, [&] (const Index_t& i) {
  ...
});
```

Using atomic_add for scatter add (27x)

```
//replace
    for (Index_t lnode = 0; lnode < 8; ++lnode) {
      Index_t gnode = elemToNode[lnode];
      domain.fx(gnode) += fx_local[lnode];
      domain.fy(gnode) += fy_local[lnode];
      domain.fz(gnode) += fz_local[lnode];
    }
//with
    for (Index_t lnode = 0; lnode < 8; ++lnode) {
      Index_t gnode = elemToNode[lnode];
      Kokkos::atomic_add(&domain.fx(gnode), fx_local[lnode]);
      Kokkos::atomic_add(&domain.fy(gnode), fy_local[lnode]);
      Kokkos::atomic_add(&domain.fz(gnode), fz_local[lnode]);
    }
```

Taking Error Checks out of Loops (8x)

```
//replace
for (Index_t i = 0; i < numElem; ++i) {
  ...
  if (domain.v(i) <= Real_t(0.0))
      MPI_Abort(MPI_COMM_WORLD, VolumeError);
}
//with
int check_error = 0;
Kokkos::parallel_for ( numElem, [&] (const Index_t& i) {
  ...
  if (domain.v(i) <= Real_t(0.0)) {
    check_error = 1;
});
if (check_error)
  MPI_Abort(MPI_COMM_WORLD, VolumeError);
```

Adding GPU Support

- Use capture by value
- Make member functions const
- Replace std::containers with other data structures and use Kokkos::malloc for allocations

Classes need const members and function markup

```
//replace
class Domain {
  ...
  Real_t &x(const Index_t idx) { return m_x[idx]; }
};
//with
class Domain {
  ...
  KOKKOS_INLINE_FUNCTION Real_t &x(const Index_t idx) const { return m_x[idx]; }
};
```

Replace std::vector with Kokkos::vector

```
//replace
class Domain {
  ...
  Kokkos::std<Real_t> m_x;
};
//with
class Domain {
  ...
  Kokkos::vector<Real_t> m_x;
};
```

Avoid reallocation of temporary buffers 28x

```
//replace
Real_t *fx_elem = Allocate<Real_t>(numElem8);
Real_t *fy_elem = Allocate<Real_t>(numElem8);
Real_t *fz_elem = Allocate<Real_t>(numElem8);
...
Release(&fz_elem);
Release(&fy_elem);
Release(&fx_elem);
//with
ResizeBuffer((numElem8*sizeof(Real_t)+4096)*3);
Real_t *fx_elem = AllocateFromBuffer<Real_t>(numElem8);
Real_t *fy_elem = AllocateFromBuffer<Real_t>(numElem8);
Real_t *fz_elem = AllocateFromBuffer<Real_t>(numElem8);
```

Reduce register pressure by separating independent calculations

```
//replace
...
xd1[..] = ..;
yd1[..] = ..;
...
CalcElemFBHourglassForce(xd1, yd1, zd1, hourgam, coefficient,
                         hgfx, hgfy, hgfz);
//with
...
xd1[..] = ..;
...
CalcElemFBHourglassForce(xd1, hourgam, coefficient, hgfx);
...
yd1[..] = ..;
...
CalcElemFBHourglassForce(yd1, hourgam, coefficient, hgfy);
...
```

Start using Views with Traits and Layout

```
//add
Kokkos::View<const Real_t*, Kokkos::MemoryTraits<Kokkos::RandomAccess>> m_c_x ;
...
KOKKOS_INLINE_FUNCTION Real_t c_x(const Index_t idx) const { return m_c_x[idx]; }
//replace
Real_t hourmodx =
       x8n[i3] * G.gamma[i1][0] + x8n[i3 + 1] * G.gamma[i1][1] +
       x8n[i3 + 2] * G.gamma[i1][2] + x8n[i3 + 3] * G.gamma[i1][3] +
       x8n[i3 + 4] * G.gamma[i1][4] + x8n[i3 + 5] * G.gamma[i1][5] +
       x8n[i3 + 6] * G.gamma[i1][6] + x8n[i3 + 7] * G.gamma[i1][7];
//with
Real_t hourmodx = 0.0;
for( int j = 0; j<8; j++)
  hourmodx += x8n(i2,j) * G.gamma[i1][j];
```

Utilize TeamPolicy where appropriate

```
//replace
Kokkos::parallel_for("CalcFBHourglass_B", numNode, KOKKOS_LAMBDA(const int gnode) {
  Real_t fx_tmp = Real_t(0.0);
  for (Index_t i = 0; i < count; ++i)
    fx_tmp += fx_elem[cornerList[i]];
  domain.fx(gnode) += fx_tmp;
//with
Kokkos::parallel_for ("CalcFBHourglass_B",Kokkos::TeamPolicy<>((numNode+127)/128,team_size,2),
  KOKKOS_LAMBDA (const typename Kokkos::TeamPolicy<>::member_type& team) {
  const Index_t gnode_begin = team.league_rank()*128;
  const Index_t gnode_end = (gnode_begin + 128<numNode)?gnode_begin + 128:numNode;
  Kokkos::parallel_for(Kokkos::TeamThreadRange(team,gnode_begin,gnode_end),[&] (const Index_t& gnode) {
    reduce_double3 f_tmp;
    Kokkos::parallel_reduce(Kokkos::ThreadVectorRange(team,count),[&](const Index_t& i,double3& tmp) {
      tmp.x += fx_elem[cornerList[i]] ;
    },f_tmp);
    Kokkos::single(Kokkos::PerThread(team), [&] () { domain.fx(gnode) += f_tmp.x ; });
  });
```

Merge Kernels

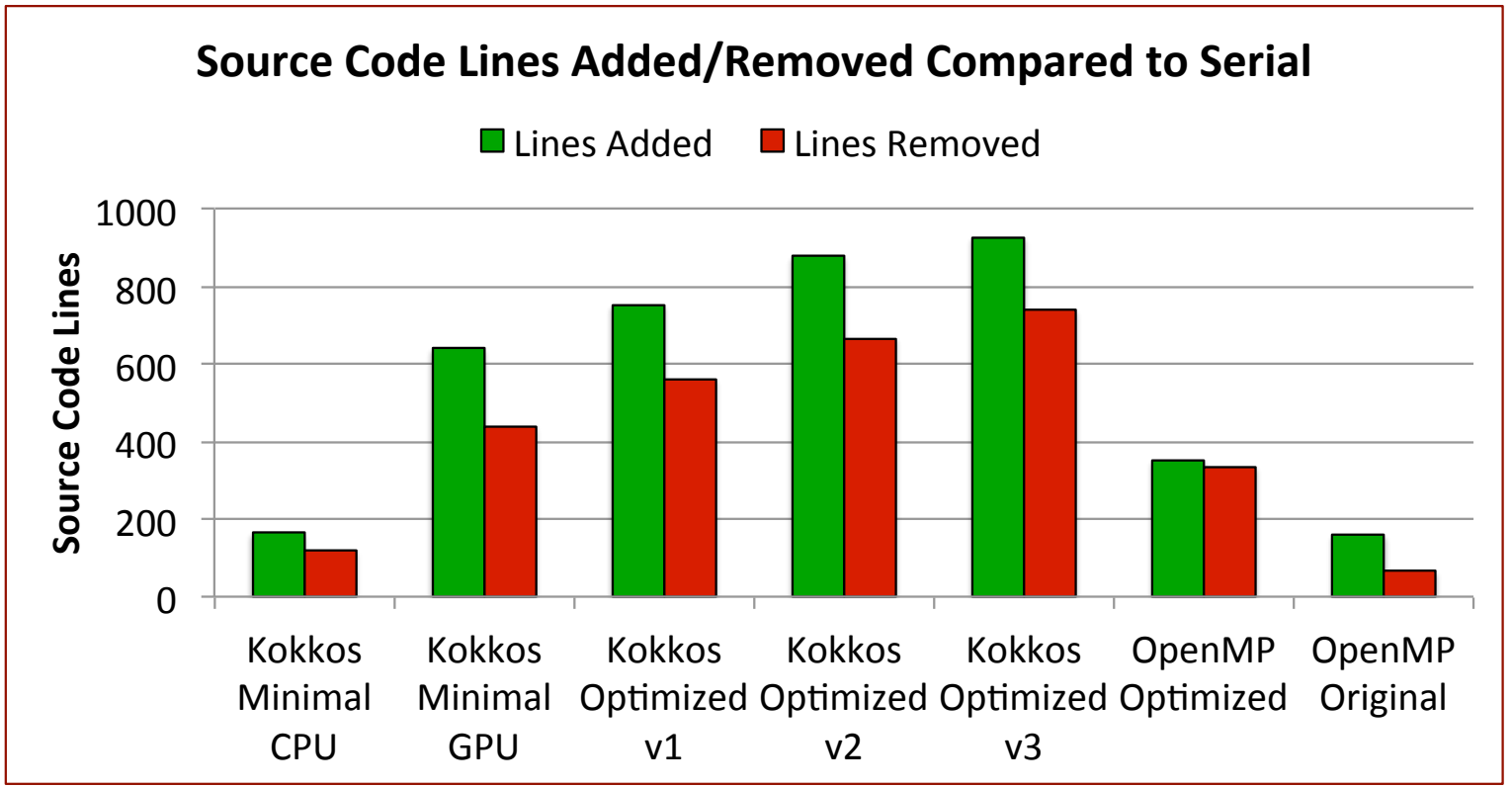
- Reduces data transfers (temporary arrays are replaced with temporary scalars)
- Reduces scheduling overhead

```
//replace
Kokkos::parallel_for("EvalEOSForElems_AA", numElemReg, KOKKOS_LAMBDA(const int i) {
  //do stuff AA
});
Kokkos::parallel_for("EvalEOSForElems_BB", numElemReg, KOKKOS_LAMBDA(const int i) {
  //do stuff BB
});


//with
Kokkos::parallel_for("EvalEOSForElems", numElemReg, KOKKOS_LAMBDA(const int i) {
  //do stuff AA
  //do stuff BB
});
```

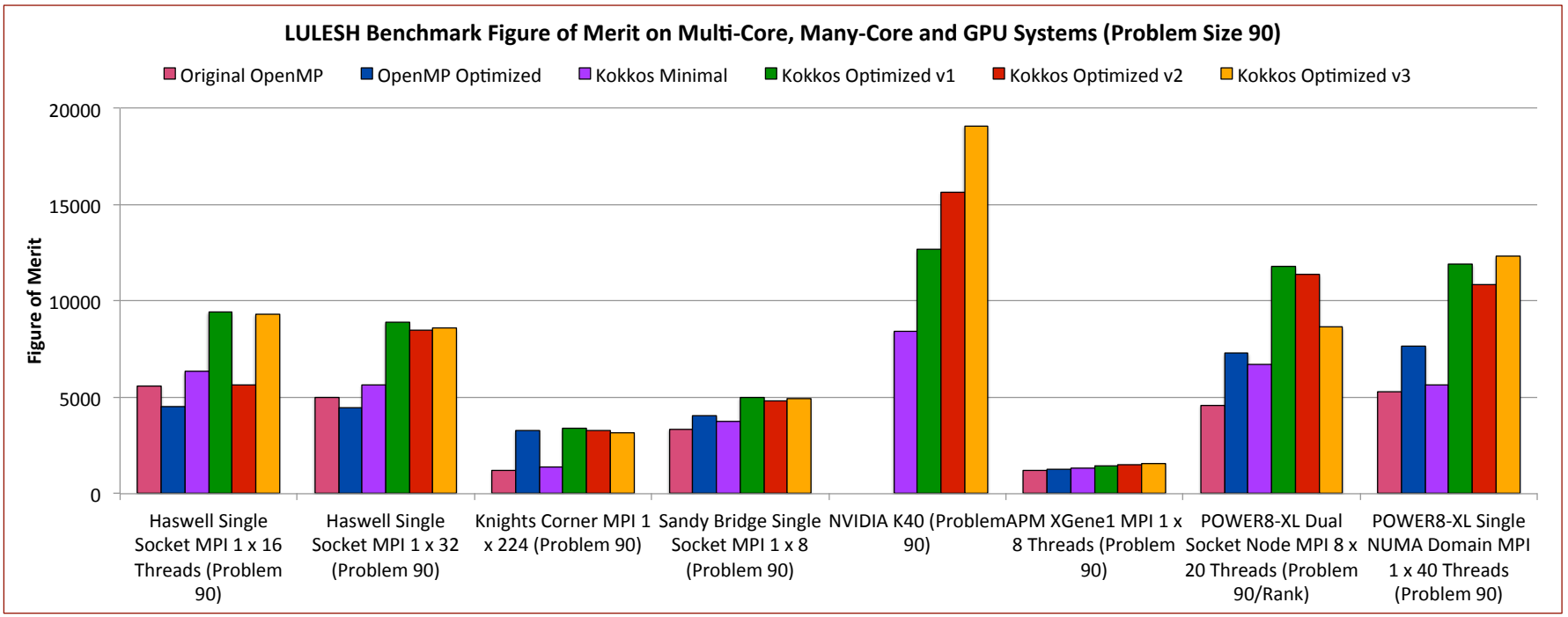
Lulesh Porting: Measuring productivity

- Count sites of modification and number of lines changed



Lulesh Porting: Performance Overview

- Preliminary data, some of it (in particular on Power) with not yet great Software stack
- Some of the testbeds show not yet understood significant performance variances

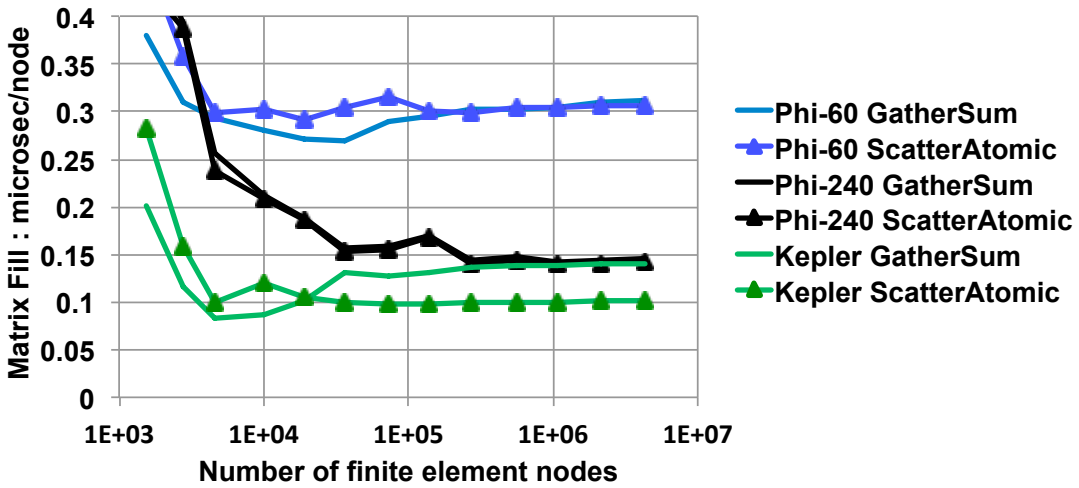


FENL: addressing Matrix assembly with Kokkos

- MiniFE++: focus on Matrix assembly
- Implement gather sum and scatter add algorithms for Matrix assembly
- Use Newton iterations to exercise it.

Expanding FENL into a miniDriver

- Utilize Trilinos Tpetra data structures
- Exercise Trilinos Solvers (including AMG)
- Allow for UQ data types
- Now: expand to use Sierra data structures for assembly, and Sierra solvers



Benefits of miniApps

- OpenSource as opposed to export controlled or even classified
- Faster turn around time: an intern can write a new version
- Often small enough to allow run in simulators.
- Little dependencies: can be exercised on new software stacks

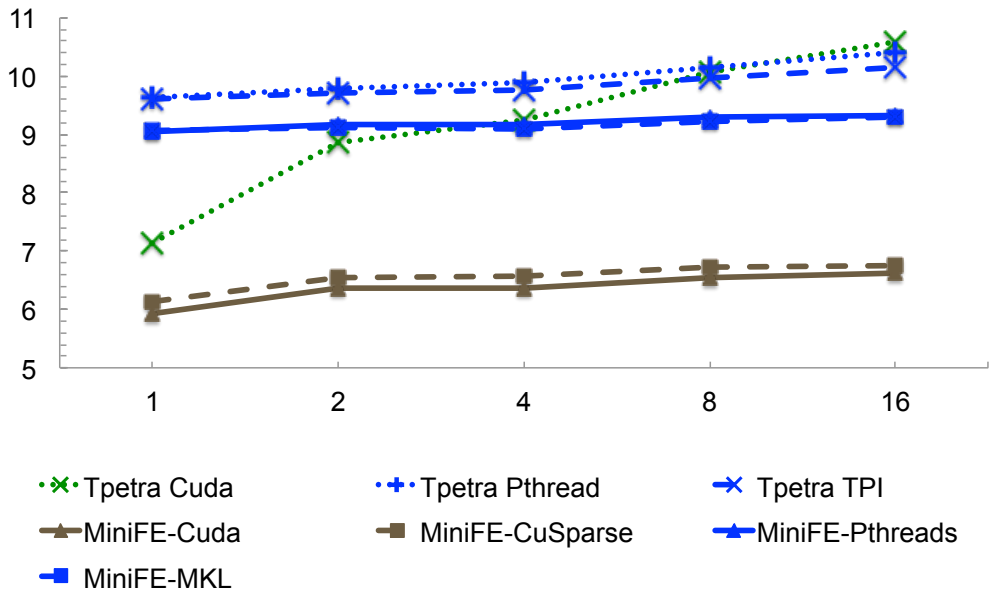
Kokkos and the AMD Kalmar Compiler

- Collaboration to develop Kokkos backend for APUs
- Use MiniApps to drive development and test results
- 40 hours ago: got Lulesh-Minimal-GPU and Lulesh-Opt-1 working
- Identified several bugs in compiler as well as new requirements to enable higher optimization levels

Evaluating pre-release versions to head of issues

- Tpetra is Trilinos 2nd generation distributed linear algebra interface
- Started to move to Kokkos in 2013
- Utilizes UVM for NVIDIA platforms to deal with complex data management issues (by ignoring them)
- Performance issues identified as compared to MiniFE which didn't use UVM - but neither requires data transfer during CG-Solve

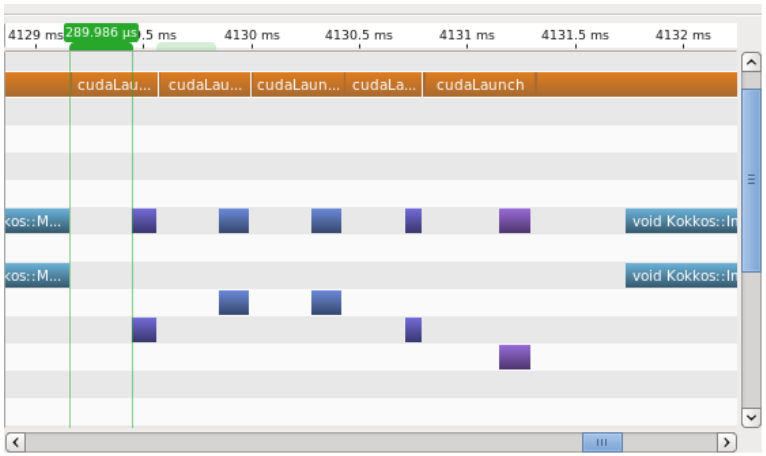
Time for CG-Solve vs number of nodes (Weak scaling problem)

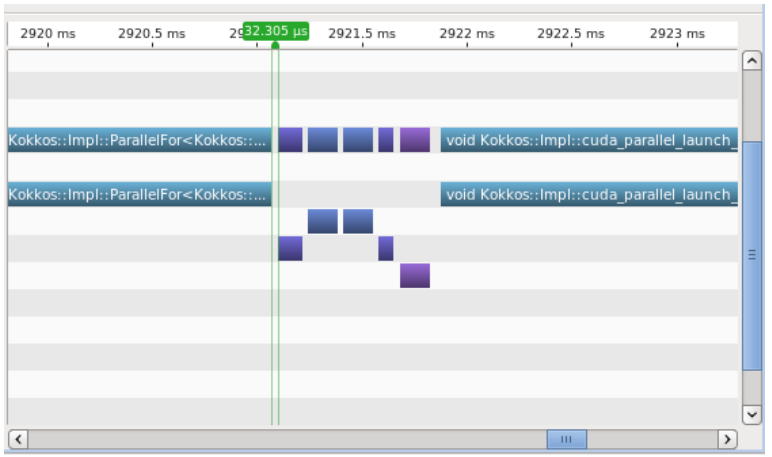


Replicate issue in MiniFE

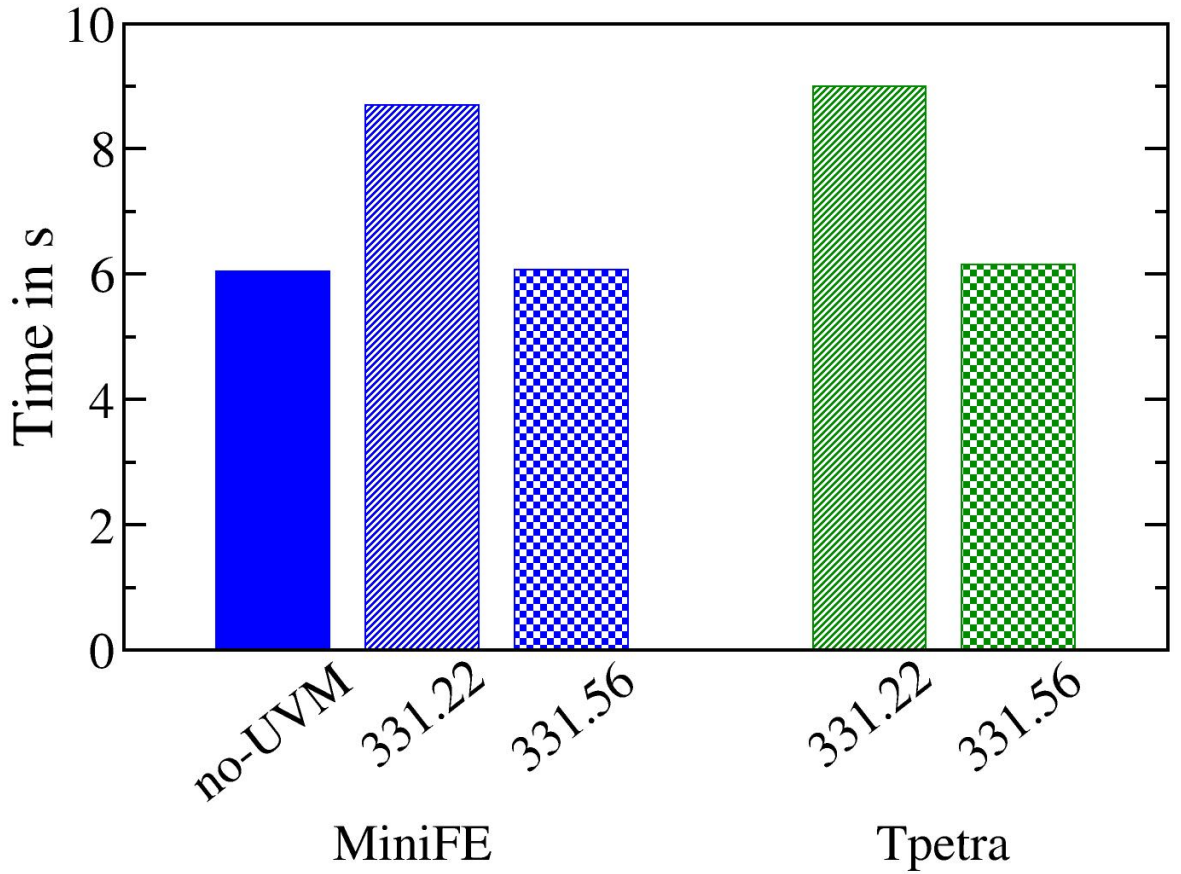
- To hard to eliminate use of UVM in Tpetra ¿ add UVM to MiniFE
- Replicate On-Node issue
- Investigate with Profiler
- Finding launch overhead unrelated to data transfer
- Send findings to NVIDIA

Profiler comparison of UVM and noUVM variant





Fix came with driver update



Summary

- Proxy Apps are an important tool of collaboration
- More nimble than real apps
- Allow for experimentation which is hard to do in production code
- Develop strategies before starting to modify production codes
- But: wider spectrum from skeleton apps to miniDrivers is needed to cover different needs

Summary

- Proxy Apps are an important tool of collaboration
- More nimble than real apps
- Allow for experimentation which is hard to do in production code
- Develop strategies before starting to modify production codes
- But: wider spectrum from skeleton apps to miniDrivers is needed to cover different needs

ProxyApps are here to stay!